Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(2,2′-Bipyridine)dichlorogold(III) nitrate

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Received 18 October 2004
Accepted 20 October 2004
Online 30 October 2004

The title compound, $[AuCl_2(C_{10}H_8N_2)]NO_3$, is layered parallel to $(\bar{1}01)$ by π–π stacking. The individual $\{\bar{1}01\}$ layers are held together by extensive C—H···O and C—H···Cl hydrogen bonding.

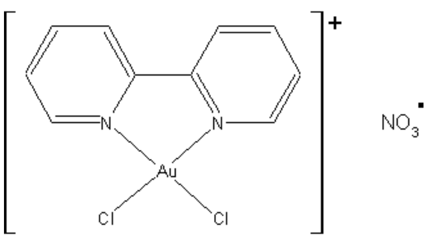
Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.008 Å
R factor = 0.026
wR factor = 0.053
Data-to-parameter ratio = 14.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

The title compound, $[Au(bipy)Cl_2]NO_3$, (I), was synthesized by reaction of the corresponding chloride with ammonium nitrate in an attempt to synthesize $[Au(bipy)(NH_3)_2](NO_3)_3$.



(I)

Compound (I) (Fig. 1) is closely related to the previously characterized $[Au(bipy)Cl_2]BF_4$ salt, (II) [Cambridge Structural Database Version 5.25 (Allen, 2002) refcode ZENFED (McInnes *et al.*, 1995)], which has the same cation. Indeed, no change is observed in the intramolecular geometry of the cation in the two structures. It should noted that, while the cation in (II) has approximate C_{2v} symmetry, this is exact in (I) by being imposed by the space group (*cf.* Fig. 1). There are significant differences in the packing between the two structures. Nitrate is a stronger donor than tetrafluoroborate and this is observed in the structure. (I) and (II) both show axial interactions to the peripheral atoms of their counter-ions, NO_3^- and BF_4^-, respectively, but these are found to be much

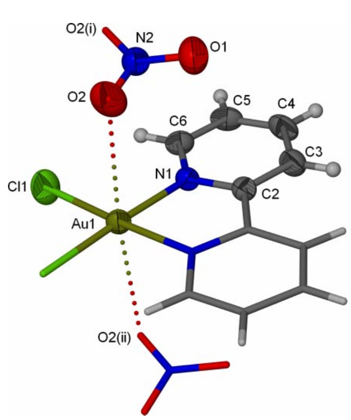


Figure 1
View of (I), shown with 50% probability displacement ellipsoids for the asymmetric unit only. [Symmetry codes: (i) $-x, y, \frac{1}{2}-z$; (ii) $1-x, y, \frac{1}{2}-z$.]

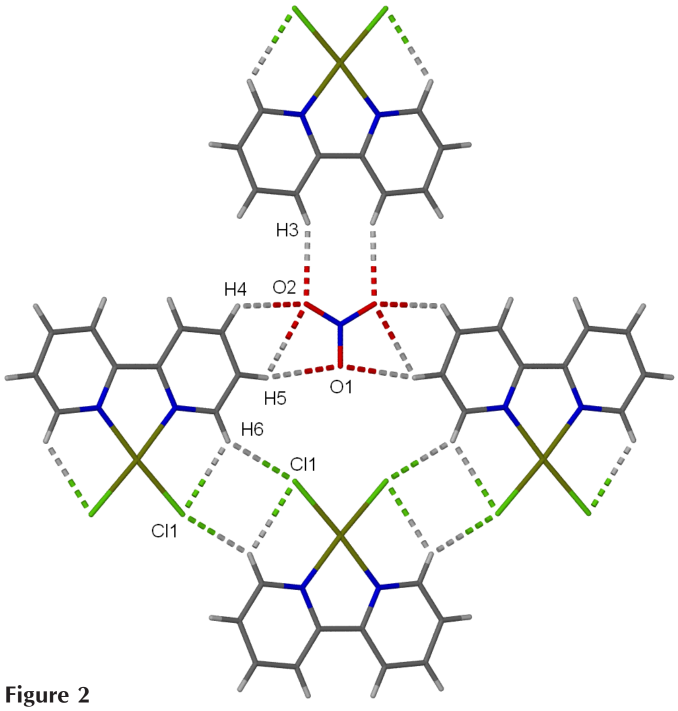


Figure 2
The short C—H···O and C—H···Cl interactions (dashed lines) in the $(40\bar{4})$ plane.

shorter in (I) than in (II): Au···O = 3.008 (5) Å *versus* Au···F = 3.165–3.781 Å.

More important are the short C—H···O and C—H···Cl interactions (Table 2) illustrated in Fig. 2. The nitrate ion is seen to be coplanar with the complex cation, except for a small twist induced by the Au···O interactions. These hydrogen bonds link cations and anions into sheets parallel to the $(\bar{1}01)$ plane. The sheets are then held together by Au···O interactions and π–π stacking between the pyridine rings, with centroid-to-centroid and plane-to-plane distances of 3.662 (3) and 3.336 Å, respectively. This is vastly different from the situation in (II), where no π–π stacking is observed and the molecules pack in a herringbone manner through C—H···F interactions, comparable to the C—H···F seen in (I), together with weaker C—H···Cl, C—H···π and Cl···π interactions.

Experimental

The title compound was produced according to an established procedure (McInnes *et al.*, 1995). In an attempt to replace the coordinated chloride with ammonia, a solution of the crude product was mixed with a concentrated solution of ammonium nitrate (4 *M*). Crystals of (I) precipitated after one day at room temperature.

Crystal data

$[AuCl_2(C_{10}H_8N_2)]NO_3$	D_x = 2.559 Mg m^{-3}
M_r = 486.06	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 6608 reflections
a = 6.9236 (2) Å	θ = 2.9–27.5°
b = 14.0458 (4) Å	μ = 12.09 mm^{-1}
c = 13.0559 (4) Å	T = 150 (2) K
β = 96.5623 (13)°	Block, pale yellow
V = 1261.44 (6) Å^3	0.30 × 0.10 × 0.05 mm
Z = 4	

Data collection

Nonius Kappa CCD diffractometer	1097 reflections with $I > 2\sigma(I)$
φ and ω scans	R_{int} = 0.071
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)	θ_{max} = 26°
T_{min} = 0.461, T_{max} = 0.544	$h = -8 \rightarrow 8$
10491 measured reflections	$k = -17 \rightarrow 17$
1247 independent reflections	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.026	$w = 1/[\sigma^2(F_o^2) + (0.0222P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.053	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.06	$\Delta\rho_{max}$ = 0.54 e Å^{-3}
1247 reflections	$\Delta\rho_{min}$ = −0.96 e Å^{-3}
88 parameters	

Table 1
Selected geometric parameters (Å, °).

Au1—N1	2.030 (4)	Au1—Cl1	2.2510 (15)
N1—Au1—N1^{ii}	80.6 (2)	N1—Au1—Cl1^{ii}	176.06 (11)
N1—Au1—Cl1	95.46 (12)	Cl1—Au1—Cl1^{ii}	88.45 (9)

Symmetry code: (ii) $1-x, y, \frac{1}{2}-z$.

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O2^{iii}	0.95	2.42	3.307 (7)	156
C4—H4···O2^{iv}	0.95	2.55	3.205 (7)	126
C5—H5···O1^{v}	0.95	2.65	3.582 (5)	167
C5—H5···O2^{iv}	0.95	2.71	3.287 (7)	120
C6—H6···Cl1	0.95	2.64	3.231 (6)	121
C6—H6···Cl1^{vi}	0.95	2.69	3.476 (5)	141

Symmetry codes: (iii) $\frac{1}{2}-x, \frac{1}{2}+y, \frac{1}{2}-z$; (iv) $x, 1-y, z-\frac{1}{2}$; (v) $-x, 1-y, -z$; (vi) $\frac{1}{2}-x, \frac{1}{2}-y, -z$.

All H atoms were constrained to have optimum geometry in the riding model, with C—H distances of 0.95 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *COLLECT* (Nonius, 1997–2000); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *HKL DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *DIRDIF*99 (Beurskens *et al.*, 1999); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *WinGX* publication routines (Farrugia, 1999).

We thank the EPSRC for funding for the purchase of the diffractometer.

References

Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.
Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Beurskens, P. T., Beurskens, G., de Gelder, R., García-Granda, S., Gould, R. O., Israel, R. & Smits, J. M. M. (1999). *The DIRDIF99 Program System*. Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
McInnes, E. J. L., Welch, A. J. & Yellowlees, L. J. (1995). *Acta Cryst.* C**51**, 2023–2025.
Nonius (1997–2000). *COLLECT*. Nonius BV, Delft, The Netherlands.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
Sheldrick, G. M. (1997). *SHELXL*97. University of Göttingen, Germany.